

Butanedioic acid, 2,2,3,3-tetrafluoro-
377-38-8 | DTXSID8059928

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.72 | 51.8 | 0.74 | 50.3 | 0.73 | 52.7 |

Model Results

Predicted value: 116 °C

Global applicability domain: Inside

Local applicability domain index: 4.21e-01

Confidence level: 6.05e-01

Nearest Neighbors from the Training Set

| | | |
|---|---|--|
| <div>Image not found</div> <div>Butanedioic acid, 2,2,3,3-tetrafluoro-</div> <div>Measured: 119</div> <div>Predicted: 116</div> | <div>Image not found</div> <div>Pentanedioic acid, hexafluoro-</div> <div>Measured: 80.0</div> <div>Predicted: 91.3</div> | <div>Image not found</div> <div>Hexanedioic acid, 2,2,3,3,4,4,5,5-octafluoro-</div> <div>Measured: 134</div> <div>Predicted: 123</div> |
| <div>Image not found</div> <div>1,5-Pentanediol, 2,2,3,3,4,4-hexafluoro-</div> <div>Measured: 79.5</div> <div>Predicted: 76.4</div> | <div>Image not found</div> <div>3,4,5,6-Tetrafluorophthalic acid</div> <div>Measured: 163</div> <div>Predicted: 167</div> | |